Tunneling spectroscopy of a macroscopic variable

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We develop a theory of the line shape for macroscopic tunneling spectroscopy and show how both spectral linewidths and line shifts are related to phenomenological dissipative coefficients for the relevant macroscopic coordinate. In the limit of weak dissipation our theory justifies a simple approximate interpretation of recent experiments on Josephson junctions; in this way macroscopic tunneling spectroscopy can be used to obtain accurate *in situ* estimates of the parameters required to calculate the absolute rate of macroscopic tunneling. Our calculations also clarify the extent to which spectroscopic experiments provide evidence for macroscopic quantum behavior.

The quantum-mechanical behavior of macroscopic systems[1] has thus far been probed by two very different types of experiment, both carried out on Josephson junctions. In the first,[2] a system is prepared in a metastable state and one measures the rate of escape from this state; quantitative comparison with quantum-mechanical predictions provides evidence that the escape proceeds by tunneling of a macroscopic coordinate. In the second,[3] one studies changes in this tunneling rate induced by an external field at frequency ω; resonances in this "tunneling spectrum" are interpreted as transitions among quantized energy levels *within* the metastable state. While macroscopic tunneling is the subject of a large theoretical literature,[4] several physical issues which arise in tunneling spectroscopy of a macroscopic coordinate have not been discussed at all:[5] How is the simple picture of transitions among quantum levels affected by dissipation? What features of the spectrum provide evidence for quantum—as opposed to classical resonant—behavior? What are the conditions for observing these quantum effects?

Here we present a theory of line shapes—the effects of dissipation—for macroscopic tunneling spectroscopy. Our analysis is confined to the limit of small dissipation and assumes that the tunneling events themselves are semiclassical, conditions which are met in the experiments of Ref. 3. We show that under these conditions—and as far as we can see, *only* under these conditions—the tunneling spectrum admits a very simple physical interpretation. In this regime both spectral line widths and line shifts are calculated; both are found to be independent of assumptions regarding the asymptotic behavior of the dissipative mechanism at frequencies far from the measurement frequency. The line shifts are "doubly small," being proportional both to the phenomenological dissipation coefficient and to the deviation of the undamped macroscopic coordinate from semiclassical behavior; this justifies an approximate interpretation of the Josephson junction experiments which neglects the line shifts altogether. The absolute strength of lines in the tunneling spectra are more difficult to interpret and especially to measure, so we shall not discuss them here.

Consider a "particle" of unit mass moving in a potential $V(q)$ having a single well separated from the continuum by a classically forbidden region (the barrier to tunneling). The coordinate q is coupled to a heat bath which generates a frequency dependent linear damping constant $\gamma(\omega)$; by this we mean that the classical Langevin equation for $q(t)$ is

$$\frac{d^2q(t)}{dt^2}+\int\frac{d\omega}{2\pi}\gamma(\omega)\int dt' e^{-i\omega(t-t')}\frac{dq(t')}{dt'}+\frac{\partial V[q(t)]}{\partial q}=F_{\rm ext}(t)+\delta F(t)\,, \tag{1}$$

where $F_{\rm ext}(t)$ is an external force and $\delta F(t)$ is chosen from a stationary Gaussian ensemble of functions with spectral density.

$$\int d\tau e^{i\omega\tau}\langle\delta F(t)\delta F(t-\tau)\rangle=2k_BT\,{\rm Re}\gamma(\omega)\,. \tag{2}$$

As a microscopic model[6] we couple $q(t)$ linearly to some generalized coordinate $X(t)$ of the bath, so that

$$H=\tfrac{1}{2}\dot q^{\,2}+V(q)+gqX+H_{\rm bath}(X)\,. \tag{3}$$

The dynamics of this model reproduce those of Eq. (1) if the heat-bath coordinate $X(t)$ responds linearly to its conjugate force and if the response function (determined by the details of $H_{\rm bath}$) is chosen as $\tilde\chi(\omega)=i\omega g^{-2}\gamma(\omega)$. Quantum mechanically this is equivalent to the statement that in the bare ($g=0$) theory $X(t)$ is a free field with the retarded propagator ($\hbar=1$)

$$\chi(t)=-i\theta(t)\langle[\hat X(t),\hat X(0)]\rangle=g^{-2}\int\frac{d\omega}{2\pi}i\omega\gamma(\omega)e^{i\omega t}\,. \tag{4}$$

We note that this program may also be implemented by writing $X(t)$ as a sum of harmonic oscillator or fermion coordinates,[7] but the essential idea behind either approach is that of linear response, as emphasized by Caldeira and Leggett.[4]

In quantizing the theory it is convenient to define energy levels ϵ_n in the well formed by $V(q)$. We do this by truncating the potential[8] with an infinite wall at some q_1 deep inside the classically forbidden region. This wall divides the entire configuration space $\{q,X\}$ into two regions and prevents tunneling out of the well. Our strategy is to solve the truncated problem perturbatively in g, and then to remove the wall and allow tunneling to occur; in the semiclassical (small $\hbar$), low dissipation limit this procedure treats the different energy scales of the problem in order of decreasing significance, as will be seen below.

The truncated problem is equivalent to the one-particle sector of

$$H_T=\sum_n \epsilon_n c_n^\dagger c_n + H_{\text{bath}}(X)+gX\sum_{m,n} q_{nm} c_n^\dagger c_m \;, \quad (5)$$

where q_{nm} are matrix elements of q between eigenstates of truncated problem and the $c_n^\dagger$ are fermion operators which create the states $|\, n\,\rangle$ of the macroscopic system. At zero temperature we are interested in the generating functional

$$\Lambda[J_n^\dagger,J_n]=\left\langle T\exp\left[-i\int dt\sum_n [J_n^\dagger(t)c_n(t)+\text{H.c.}]\right]\right\rangle \;, \quad (6)$$

where the $J_n^\dagger, J_n$ are Grassman variables and $\langle \cdots \rangle$ denotes a vacuum expectation value. This functional gives Green's functions which describe the dynamics of a system suddenly created in state $|\, n\,\rangle$, and from these Green's functions we can extract the energies and lifetimes of the states by standard arguments. This procedure generalizes to finite temperature provided that our expectation value is always taken in a state of zero fermions.

Passing to the interaction representation we can write Λ as a functional integral and integrate out the coordinates $X(t)$, essentially following the influence functional formalism[9] but for the generating functional rather than for the propagator itself; this procedure can of course also be carried out for the individual Green's functions. The result is exactly equivalent to a pure fermion system with effective energy-dependent pairwise interactions defined by

$$\int dt H_{\text{int}}^{\text{eff}}(t)=-\frac{i}{2}\sum_{n,m,k,l} q_{nm}q_{kl}\int dt\int dt'\int\frac{d\omega}{2\pi}\,|\,\omega\,|\,\gamma(\omega)e^{-i\omega(t-t')}c_m^\dagger(t)c_k^\dagger(t')c_n(t)c_l(t') \;. \quad (7)$$

From this effective interaction we construct a diagrammatic perturbation theory in the usual way. The small parameter for this expansion is $\alpha\sim\gamma q^2/\hbar$, where γ is a typical value of $\gamma(\omega)$ and q is a typical value of q_{nm}. Since $q^2\sim\hbar/2\omega$ we see that $\alpha\sim\gamma/\omega=1/Q$, where Q is the quality factor of classical small-amplitude oscillations in the metastable well.

Our goal is to calculate, to lowest order in the dissipation, the shift and broadening of energy levels in the metastable well; we emphasize that the connection to tunneling will be made below only when we remove the barrier at q_1. The relevant quantities are the diagonal terms in the self-energy matrix evaluated on energy shell, since both off-diagonal and off-shell effects are of higher order in the dissipation. We obtain

$$\Sigma_{nn}(\epsilon_n)=\lim_{\delta\to 0^+}\int_0^\infty\frac{d\Omega}{2\pi}\gamma(\Omega)\Omega\sum_m\frac{|\,q_{nm}\,|^2}{\epsilon_n-\epsilon_m-\Omega+i\delta} \;. \quad (8)$$

The imaginary part of Σ_{nn} can be readily evaluated for arbitrary frequency dependent dissipation,

$$\text{Im}\Sigma_{nn}(\epsilon_n)=-\sum_m |\,q_{nm}\,|^2\theta(\epsilon_n-\epsilon_m)(\epsilon_n-\epsilon_m)\gamma(\epsilon_n-\epsilon_m) \;. \quad (9a)$$

The real part is only slightly more complicated; for instance in the case of Ohmic dissipation with cutoff, $\gamma(\omega)=\gamma\theta(\omega_c-|\,\omega\,|)$,

$$\text{Re}\Sigma_{nn}(\epsilon_n)=-\frac{\gamma}{\pi}\sum_m |\,q_{nm}\,|^2(\epsilon_n-\epsilon_m)\ln\left|\frac{\omega_c}{\epsilon_n-\epsilon_m}\right| \;. \quad (9b)$$

If the states $\{|\,n\,\rangle\}$ were precisely harmonic oscillator eigenstates $[\epsilon_n=\hbar\omega_0(n+\frac{1}{2})]$, the lifetime of the nth state would be, for arbitrary $\gamma(\omega)$, $\tau_n\equiv[2\,\text{Im}\Sigma_{nn}(\epsilon_n)]^{-1}=[n\gamma(\omega_0)]^{-1}$, and the shift of the (real part of the) energy $\Delta\epsilon_n\equiv\text{Re}\Sigma_{nn}(\epsilon_n)$ would be independent of n. For instance, if the dissipation were Ohmic, $\Delta\epsilon_n=(\gamma/2\pi)\ln(\omega_c/\omega_0)$. Whenever $\Delta\epsilon_n$ is independent of n changes in the observable energy differences, $\Delta\epsilon_{n\to m}=\Delta\epsilon_n-\Delta\epsilon_m$, vanish. In the small $\hbar$ limit the low lying states are always well described by harmonic oscillator states, so we conclude that the shift in level spacing due to interaction with the heat bath is of second order in $\hbar$.

The energy shift produced by an Ohmic heat bath interacting with a harmonic oscillator is logarithmically divergent as the cutoff goes to infinity. While this logarithm is not, in itself, alarming, since it is n independent, its presence alerts us to the necessity of showing that similar divergences do not occur in observable quantities when the full anharmonic potential is considered. Energy-level differences will be independent of the cutoff and hence immune to the divergence if $\sum_k |\,q_{nk}\,|^2(\epsilon_n-\epsilon_k)$ is independent of n. Summing over the complete set of states we have

$$\sum_k |\,q_{nk}\,|^2(\epsilon_n-\epsilon_k)=\tfrac{1}{2}\langle\, n\,|\,[[HT,q],q]\,|\,n\,\rangle \;,$$

so that

$$\sum_k |\,q_{nk}\,|^2(\epsilon_n-\epsilon_k)\sim[p,q]=\text{constant} \;,$$

as required.

As an explicit example we consider the potential

$$V(q)=\tfrac{1}{2}\omega_0^2q^2+g_3q^3+g_4q^4+\cdots$$

and calculate energy-level shifts perturbatively in the couplings g_3,g_4. This is in fact a systematic semiclassical expansion for an *arbitrary* potential, since terms $\sim g_nq^n, n>4$, contribute only at higher order in $\hbar$. In the absence of interactions with the heat bath we have energy levels

$$\epsilon_n=\hbar\omega_0\left[1+\hbar\left[\frac{3g_4}{2\omega_0^3}-\frac{15g_3^2}{4\omega_0^5}\right]+\cdots\right](n+\tfrac{1}{2})$$
$$+\hbar^2\omega_0\left[\frac{3g_4}{2\omega_0^2}-\frac{15g_3^2}{4\omega_0^5}+\cdots\right]n^2+\text{constant}\ ,$$

and we find the observable line shifts

$$\Delta\epsilon_{n\to m}=(n-m)\left[-\frac{2\gamma}{\pi\omega_0}\right]\hbar^2\omega_0$$
$$\times\left[\frac{3g_4}{\omega_0^3}-\frac{g_3^2}{\omega_0^5}(\tfrac{15}{2}-\ln 2)\right]+\cdots\ . \qquad (10)$$

Thus we see that the "dissipative Lamb shift" $\Delta\epsilon_{n\to m}$ is explicitly of order $\hbar^2$, as promised, and is small both by a factor $1/Q$ and by the smallness of the anharmonicity g_3,g_4 (which is equivalent). Finally, since $\Delta\epsilon_{n\to m}\sim(n-m)$, the dissipative Lamb shift is at this order just a renormalization of the frequency ω_0; this does not persist to order $\hbar^3$, but these are typically very small corrections.

To connect the dynamics within the metastable well to tunneling spectroscopy requires that we remove the artificial barrier introduced above. This can be done rigorously using the path decomposition expansion[8] to give a self-energy matrix with elements on the order of the tunneling rates $\Gamma\sim\omega_0e^{-S/\hbar}$, where S is the minimum action for tunneling through the barrier. In semiclassical situations $S\gg\hbar$ so this is by far the smallest energy scale in the problem. Several points should now be noted.

(1) Since the tunneling rates are the smallest energy scale in the problem they contribute only diagonal and imaginary parts to the self-energy, $\Sigma_{nm}\sim-i\delta_{nm}\Gamma_n$.

(2) The Γ_n are strictly the self-energies obtained upon removing the barrier from the full problem with dissipation; they must thus already include corrections due to damping.[4]

(3) To get reliable estimates of Σ we must be careful to include many states in the well even at low temperatures. This is due to the fact that if we keep only the lowest n levels we necessarily make errors in describing the coupling to heat bath modes at frequencies $\Omega\sim n\omega_0$. Since it precisely those modes with $\Omega\sim\omega_0$ which dominate the dynamics, it is clear that n must be large compared to 1.

(4) The calculation outlined above is easily generalized to finite temperature by replacing the free propagator of the heat-bath coordinate with its finite-temperature form. The result is to introduce Bose occupation factors in Eqs. (9); thus the lifetime of each state decreases when $k_BT\geq\hbar\omega_0$.

(5) Since $\Gamma_n\ll|\Sigma_{nn}|$ we can interpret Γ_n as the decay rate from state $|n\rangle$ out of the well and $\mathrm{Im}\Sigma_{nn}$ as the decay $n\to\{n'\}$ within the well. In fact this inequality must be satisfied if the notion of tunneling at fixed temperature is to make sense; if it is not satisfied then the system can tunnel before it equilibrates and hence the decay rate is sensitive to the initial preparation of the state within the metastable well.

(6) In general the rate at which an external field induces transitions among the states in the metastable well can be written in terms of multipoint Green's functions, as can the field-induced change in the tunneling rate. In a many-body system these multipoint Green's functions can have poles which are not derivable from those of the two-point functions, but in our problem these collective excitations do not exist—only one "particle" is present at any one time. As a result we can obtain the transition rates by simple perturbation theory using the energy levels and lifetimes derived above, and this will give the correct spectral *shape* although not necessarily the correct absolute rates. For an external field which couples linearly to q, transitions $n\to m$ occur at rates

$$\nu_{nm}\sim\int\frac{d\omega}{2\pi}I(\omega)\frac{|q_{nm}|^2[1/\tau_n+1/\tau_m]}{(\omega+\epsilon_n-\epsilon_m+\Delta\epsilon_{n\to m})^2+(1/\tau_n+1/\tau_m)^2}\ , \qquad (11)$$

where $I(\omega)$ is the spectral density of the field. Similarly, the field-induced tunneling rate out of the well is of the form

$$\Delta\Gamma\sim\sum_{n,m}P_n\nu_{nm}(\Gamma_m-\Gamma_n)/\gamma_m\ , \qquad (12)$$

where P_n is the thermal occupation probability of state $|n\rangle$ and γ_m is an effective decay rate; in general $\gamma_m\sim1/\tau_m$. Again, these arguments give the line shape but not the absolute intensities. These intensities depend in detail on the potential, however, and are extremely difficult to measure.

(7) At high temperatures we expect that the dynamics are fully classical. In this regime there may still be classical resonances at integral multiples of the small oscillation frequency ω_0; resolvable resonances of this sort do not imply quantum behavior. The only clear evidence of quantum behavior that can be seen in the tunneling spectrum involves the resolution of lines spaced by less than ω_0, e.g., the $0\to1$ and $1\to2$ lines which are separated by $\sim\hbar^2\omega_0^2/V_0$, with V_0 a typical scale in the potential $V(q)$. From the results above regarding temperature-dependent linewidths we estimate that these quantum resonances merge into a broad asymmetric smear[10] above

$T \sim (\hbar\omega_0/k_B)Q(\hbar\omega_0/V_0)$. In general, this temperature may be quite different from the naive prediction that systems are classical above $T \sim \hbar\omega_0/k_B$.

We conclude that because the dissipative Lamb shift is so small, macroscopic tunneling spectroscopy yields spectral lines whose position can be interpreted as the differences among energy levels in the metastable well and whose widths may be identified with rates of dissipative transitions among these levels as in the standard Breit-Wigner picture. This is not an obvious conclusion, and in particular depends critically on the combination of small damping and semiclassical motion. We also conclude that tunneling spectra depend only on $\gamma(\omega)$ at the frequencies of the observed transitions and hence this spectroscopy is quite insensitive to the form of the dissipation. The simple interpretation which can be given to macroscopic tunneling spectroscopy suggests that it will provide a very accurate method for *in situ* determination of some of the parameters required for quantitative calculations of macroscopic quantum effects. Finally, from the results discussed here it is clear that the observation by Martinis *et al.*[3] of resolved $0 \rightarrow 1$ and $1 \rightarrow 2$ transitions—with a splitting in agreement with that calculated for the undamped, truncated problem—does indeed provide evidence for the validity of quantum mechanics on a macroscopic scale.

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